Journal of Computational and Applied Mathematics 226 (2009) 319–330

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Discrete-analytical methods for the implementation of variational principles in environmental applications

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ARTICLE INFO

MSC:
58E30
76R99
49Q12
81T80
65M06
65M32
65N99
65K10

Keywords:
Variational principle
Convection-diffusion
Monotonic scheme
Discrete-analytical approximation
Numerical environment modelling
Adjoint sensitivity problem
Direct and inverse modelling

ABSTRACT

A new method of constructing numerical schemes on the base of a variational principle for models including convection-diffusion operators is proposed. An original element is the use of analytical solutions of local adjoint problems formulated for the operators of convection-diffusion within the framework of the splitting technique. This results in numerical schemes which are absolutely stable, monotonic, transportive, and differentiable with respect to the state functions and parameters of the model. Artificial numerical diffusion is avoided due to the analytical solutions. The variational technique provides strong consistency between the numerical schemes of the main and adjoint problems. A theoretical study of the new class of schemes is given. The quality of the numerical approximations is demonstrated by an example of the non-linear Burgers equation. These new schemes enhance our variational methodology of environmental modelling. As one of the environmental applications, an inverse problem of risk assessment for Lake Baikal is presented.

1. Introduction

A feature of environmental modelling primarily consists of the fact that a wide range of processes, with different time-space scales and many factors of natural and man-made origin should be considered in these models. Besides, for the goals of environmental prediction and design, it is necessary to take into account various criteria and restrictions. Naturally, observational data and all a priori accessible information should also participate in the calculations whenever it is possible. Therefore, the modelling system should be built in such a way that it provides a combination of a general view over the problem, with detailed descriptions of the processes under study. The variational approach as a mathematical tool gives the possibility of organising the appropriate comprehensive modelling technology.

The preconditions for this have already been established by now. The mathematical foundation of variational principles for the investigation of partial differential equations was made in [11,10]. A way of constructing finite-difference numerical schemes for equations of mathematical physics with the help of integral identities was proposed in [10]. The methods of numerical modelling with the use of adjoint equations for complex systems, including atmospheric and oceanic problems were developed in [12,13]. The concept and methodology of the application of variational principles for the construction of adjoint sensitivity methods for non-linear models and goal functionals of general type were presented in [17]. The organisation of the functionals, integral identities and the structure of the algorithms were given by examples of atmospheric dynamics. With the help of this methodology, a 4D variational data assimilation problem on the base of a hemispheric

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doi:10.1016/j.cam.2008.08.018

model was first solved in 1976 [20]. The algorithms and the results of calculations carried out for the adjoint sensitivity functions were presented at the Joint UITAM/IUGG International Symposium on Monsoon dynamics in Delhi (1977) [16]. The development of methods for environmental problems was continued in [14,15]. A detailed description of the variational methods for the construction of numerical models, sensitivity theory methods, and organisation of numerical modelling for the atmosphere, ocean and transport of pollutants were given in [18]. Numerous applications of the methodology to the joint models related to the dynamics and air quality were described in [21]. In the last two decades, variational technology became very popular. A great number of the recent papers of many authors is devoted to the development of different adjoint sensitivity methods and their applications. A review of these approaches is given in [5].

Let us shortly describe our environmental modelling methodology. The idea is as follows. All objects of the modelling system (models of processes, criteria, restrictions, available data) are combined by means of a metric. In addition to the model state variables, the unknown adjoint functions are introduced at this stage. The objects are presented in a condensed form as an extended functional constructed by variational principles. The reason for doubling the variables, is to obtain an instrument for calculation of the adjoint sensitivity functions. The latter demands the solutions of the main and adjoint problems. These problems are generated by means of the stationary conditions for the extended functional with respect to the variations of both the state and adjoint functions. Relations between the goal functional variations and those of characteristics on external degrees of freedom are constructively realised by the adjoint sensitivity theory algorithms. The feedback from the goal functionals and restrictions to model parameters and sources is organised on the given criteria via sensitivity functions. To realise this environment modelling methodology, the universal algorithm of direct and inverse modelling was developed in [18,19,24].

There is no doubt that variational principles are a multipurpose and universal tool for modelling. However, possessing many preferences, they are in need of eliminating at least two essential constructive drawbacks. The first one is the absence of unconditionally monotonic approximations of the required accuracy. The second is an enlargement of grid patterns of the finite-difference discrete operators used for the approximation of differential operators within integral identities.

In this paper, the main attention is paid to new schemes for models having convective-diffusive operators. The variational approach is applied for their construction that allows us to obtain *optimal* numerical schemes for the realisation of the models in forward and adjoint modes. In particular, a new method of discrete-analytical approximations is developed. It results in schemes possessing the properties of absolute stability, monotonicity, and transportivity. The advantage of the approach is that the discrete-analytical methods maintain the above mentioned properties, due to the analytical solutions of the local adjoint problems that use the parameters of the carrying flow *only*. Owing to analytical solutions, the artificial numerical diffusion is avoided in the schemes. They do not use the procedures of numerical flux correction that are inherent in the commonly used numerical schemes such as TVD [8], Smolarkiewicz [31], Bott [3], Van Leer [32] and the others. Schemes with monotonisators are mostly quite acceptable for direct modelling in spite of having some drawbacks. As mentioned in [1] and discussed in details in [7], the artificial monotonisation procedures generate non-linear effects of self-limiting diffusion that are non-proper, for instance, for the real pollution transport processes. The matter is that own self-limiting diffusion may be generated for each particular constituent. As a consequence, this may distort the true evolution of their joint behaviour. As a result, the transformation operator gets inconsistent information for defining air quality. Besides, such schemes can be a considerable obstacle for organising the inverse methods based on adjoint problems, because the latter should be strictly consistent with the direct problems. Here we enhance the variational methodology by improving the quality of basic numerical schemes. It seems that we succeeded in overcoming the above mentioned demerits.

2. System organisation of environmental modelling

In this section we shortly present the mathematical tools that are the base of the concept of environmental modelling being developed by us.

2.1. Principles for constructing numerical models

To solve environmental protection problems, we need some basic elements: models of processes, models of observation, and functionals for the organisation of modelling methods, data assimilation, environmental prognosis and design. The processes mentioned above are described on different scales by the models of hydrodynamics in the climatic system, by models of transport and transformation of humidity, chemically and optically active contaminants—gases and aerosols. The influence of natural and man-made factors is taken into account in the source terms of the models.

To describe the processes and their corresponding models, we define the objects: (1) the state functions $\vec{\varphi} = \{\varphi_i, i = \overline{1, n_s}\} \in Q(D_t)$; (2) the model parameters $\vec{Y} = \{Y_i, i = \overline{1, N}\} \in R(D_t)$; (3) the adjoint functions $\vec{\varphi}^* = \{\varphi_i^*, i = \overline{1, n_a}\} \in Q^*(D_t)$. Here D_t is the domain of the space-time co-ordinates, $D_t = D \times [0, \bar{t}]$; D is the domain of space variables $\vec{X} = (X_1, X_2, X_3)$, $[0, \bar{t}]$ is the time interval; $Q(D_t)$ is the space of the state functions satisfying the conditions at the boundary Ω_t of the domain D_t. The height z or pressure p is usually taken as the vertical co-ordinate X_3. They are the base for the modified co-ordinates following the Earth's topography. The domain D may be of any scale from global to local. The functional space $Q^*(D_t)$ is adjoint with respect to the space of the state functions $Q(D_t)$; $R(D_t)$ is the space of the admissible values of parameters. The structure of the corresponding components of vector-functions $\vec{\varphi}$ and $\vec{\varphi}^*$ is identical, but their

information content is different. In our constructions, the adjoint functions are introduced for organisation of variational principles, and design of optimal numerical schemes.

The models for the given class of problems can be written in the operator form:

$$\tilde{L}(\vec{\varphi}) \equiv B\frac{\partial \vec{\varphi}}{\partial t} + G(\vec{\varphi}, \vec{Y}) - \vec{f} = 0, \tag{1}$$

where B is a diagonal matrix; $G(\vec{\varphi}, \vec{Y})$ is a non–linear matrix operator acting on different components of the state functions; $\vec{f}$ is the source term. Here we do not intend to describe all the elements of the model set in detail. Let us consider only those models from the complex that are directly connected with the distributions of heat, humidity, optically and chemically active substances in the atmosphere. Their background is the coupled system of n_s balance equations

$$L(\vec{\varphi}) \equiv \frac{\partial \pi\varphi_i}{\partial t} + \mathrm{div}(\pi(\varphi_i\vec{u} - \mu_i \mathrm{grad}\varphi_i)) + \pi(D_i(\varphi_i) + (H(\vec{\varphi}))_i - f_i) = 0 \tag{2}$$

and the continuity equation in the form

$$\frac{\partial \pi}{\partial t} + \mathrm{div}\pi\vec{u} = 0. \tag{3}$$

Here the components of the vector-function φ_i describe the potential temperature, mixing ratios for humidity characteristics, concentrations of constituents, $\vec{f} = \{f_i(\vec{X}, t),\ i = \overline{1, n_s}\}$ is the source of heat, humidity and pollutants, $\vec{u} = (u_1, u_2, u_3)$ is the velocity vector, $\mu_i = \{\mu_1, \mu_2, \mu_3\}_i$ is the diagonal tensor of the turbulent exchange coefficients for the substance φ_i, $(H(\vec{\varphi}))_i$ is a non–linear matrix operator describing the local transformation processes of the corresponding substances, $D_i(\varphi_i)$ are the operators presenting the processes of deposition and removing the substances that were not taken into account in the operators of transformation. In all these models the advective-diffusive operator is included. In the continuity equation (3) π, is a non-negative function. Its essence depends on the atmospheric model type and on the choice of the co-ordinate system in (1) as well. All the necessary elements belonging to the hydrodynamic background for the models (2) are calculated from the corresponding atmospheric models agreed with (2), by means of the variational principle, in terms of integral identities and their sum analogues. The functions $\vec{u}$, π, μ_i, f_i and input data of initial and boundary conditions are included in the parameter vector $\vec{Y}$; deposition velocities of particles u_{d_i} are taken into account in the vertical component of the velocity vector u_3.

The initial conditions and model parameters at $t = 0$ are written in the form: $\vec{\varphi}^0 = \vec{\varphi}^0_a(\vec{X})$, $\vec{Y} = \vec{Y}_a(\vec{X}, t)$, where $\vec{\varphi}^0_a$ and $\vec{Y}_a$ are a priori estimates of initial fields $\vec{\varphi}^0$ and parameters $\vec{Y}$. Boundary conditions for model closure is the consequence of the physical content of the problem under study. Let their general form be

$$\left\{\gamma\mu_n\frac{\partial\varphi}{\partial n} = \beta\varphi - q;\ \left(\varphi = \beta^{-1}q,\ \text{if}\ \gamma = 0\right)\right\}_i, \quad i = \overline{1, n_s},\ (\vec{X}, t) \in \Omega_t, \tag{4}$$

where $\{\gamma \geq 0, \beta \geq 0, q\}$ are the parameters depending on the state of the carrying flow and also on the properties of the underlying surface; n is the external normal vector to the boundary Ω_t. This is the Dirichlet condition if $\gamma = 0$. If $\gamma = 1$, these are the conditions of the second or the third type: Neumann's ($\beta = 0$) and Robin's ($\beta \neq 0$). The values of parameters are adaptively defined in dependence on the problem features and the character of the process evolution.

2.2. Variational form of the problem statement

In addition to the differential statement of the problem, let us introduce the variational form of the model (1)–(4) as the integral identity

$$I(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) \equiv \int_{D_t} (L(\vec{\varphi}), \vec{\varphi}^*)\,\mathrm{d}D\mathrm{d}t = 0. \tag{5}$$

The identity (5) is built by taking into account the boundary and initial conditions, so that the functional (5) changes into the equation of the energy balance of the system if $\vec{\varphi}^* = \vec{\varphi}$ is substituted. Fulfilling all the necessary transformations in (5), we finally get the integral identity for the model (2)–(4) in the form

$$I(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) \equiv \sum_{i=1}^{n_s}\left\{(\Lambda\varphi, \varphi^*)_i + \int_{D_t}(D_i(\varphi_i) + (H(\vec{\varphi}))_i - f_i)\varphi_i^*\pi\,\mathrm{d}D\mathrm{d}t\right\} = 0. \tag{6}$$

Here

$$(\Lambda\varphi, \varphi^*)_i \equiv \int_{D_t}\left\{\frac{\partial\pi\varphi_i}{\partial t} + \mathrm{div}(\pi(\varphi_i\vec{u} - \mu_i\mathrm{grad}\varphi_i)) + \pi d_i\varphi_i\right\}\varphi_i^*\mathrm{d}D\mathrm{d}t, \tag{7}$$

and d_i are the parameters explicitly defined in the operators of substance transformation and deposition.

2.3. The functionals as generalised characteristics of the processes

To formulate the variational principles, let us introduce, additionally to (5)–(7), a set of functionals describing the generalised characteristics of the processes and the mathematical models. From the computational viewpoint, if there is a great number of internal and external degrees of freedom in the models, the optimal control, design, and inverse modelling methods are more adaptive to operations with the global (integral) criteria, and characteristics than with those of distributed and local types. Therefore, we define the set of such characteristics by means of the functionals of general form

$$\Phi_k(\vec{\varphi}, \vec{Y}) = \int_{D_t} F_k(\vec{\varphi}, \vec{Y}) \chi_k(\vec{X}, t) \mathrm{d}D\mathrm{d}t, \quad k = \overline{1, K},\ K \geq 1, \tag{8}$$

where $F_k(\vec{\varphi}, \vec{Y})$ are the functions of the given form defined on $Q(D_t) \times R(D_t)$ and differentiable with respect to the state functions and parameters of the model, $\chi_k \geq 0$ are the weight functions, $\chi_k \in Q^*(D_t)$; $\chi_k \mathrm{d}D\mathrm{d}t$ are the corresponding Radon's or Dirac's measures in D_t [30]. Different generalised, distributed, and local characteristics of the system behaviour, ecological restrictions on the environment quality, the results of observations of different kinds, criteria for control and design, model quality criteria can be described by means of the functionals (8) with a proper choice of the functions $F_k(\vec{\varphi}, \vec{Y})$ and χ_k [23]. The variational principles are formed on the base of the integral identities (5)–(7) and extended functionals

$$\tilde{\Phi}_k(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = \Phi_k(\vec{\varphi}, \vec{Y}) + I(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*). \tag{9}$$

2.4. Construction of the discrete model analogues

The variational forms of (5) and (9) serve as the base for construction of the discrete approximation of the model. To build them, the grid domain D_t^h is introduced in D_t, and the discrete analogues of the corresponding functional spaces $Q^h(D_t^h)$, $Q^{*h}(D_t^h)$, $R^h(D_t^h)$ are defined in it. Then (5) and (9) are approximated by the sum analogues

$$I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = 0, \quad \vec{\varphi} \in Q^h(D_t^h), \vec{\varphi}^* \in Q^{*h}(D_t^h), \vec{Y} \in R^h(D_t^h), \tag{10}$$

$$\tilde{\Phi}_k^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = \Phi_k^h(\vec{\varphi}, \vec{Y}) + I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*). \tag{11}$$

The upper index h denotes the discrete analogue of the object. Discretisation of all functionals is made with the use of weak approximation, splitting, and decomposition methods. To obtain the splitting schemes, the integrals in time are approximated by the cubature formulas within the fractional steps. The different parts of the general operator are taken at the separate fractional steps. Numerical schemes for the forward version of the model (1) are obtained from the stationary conditions for the functional $I^h(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*)$ with respect to the arbitrary and independent variations of the grid components $\vec{\varphi}^*$ at the points of the grid domain D_t^h. The numerical schemes for the adjoint version are obtained from the stationary conditions for the functionals (11) to the variations of the grid components $\vec{\varphi} \in Q^h(D_t^h)$ [18]. The cubature formulas for all objects are harmonised in the discrete analogues of functional spaces.

2.5. The additive form of the integral identity

The usage of the variational principles for the approximation of the integral identity and the extended functionals in combination with decomposition and splitting methods, allows us to present the complex, multidimensional problems as a set of one-dimensional subproblems. Let the model operator and the source function admit the additive forms

$$L\varphi = \sum_{\alpha=1}^{r} L_\alpha \varphi, \qquad f = \sum_{\alpha=1}^{r} f_\alpha, \quad r \geq 1, \tag{12}$$

where r is a parameter chosen in accordance with the goals of the study. Then the identity (5) can be rewritten as

$$I(\vec{\varphi}, \vec{Y}, \vec{\varphi}^*) = \int_{D_t} \left(\frac{\partial \vec{\varphi}}{\partial t} + \sum_{\alpha=1}^{r} \left(L_\alpha \vec{\varphi} - \vec{f}_\alpha \right) \right) \vec{\varphi}^* \mathrm{d}D\mathrm{d}t = 0. \tag{13}$$

It is convenient to take $r = 4$ for the problem (2)–(4). In this case, the first three terms present convective-diffusive operators along spatial co-ordinates, and the fourth one describes transformation processes. The methodology for the construction of numerical models and splitting schemes with the help of the variational principle is presented in [18].

Here, we improve the methodology by using a new hybrid technology of discrete-analytical approximations. The technology will be explained through the example of a convection-diffusion problem. As we take advantage of the splitting method, all basic constructions will be shown for the one-dimensional case. The extension to many dimensions is straightforward.

2.6. Decomposition of integral identity

To describe the main constructions within the interval $t_{j-1} \le t \le t_j$, let us consider the time-discrete fragment of the integral identity (13) that contains the advective-diffusive operator for one component of the state vector in the x-direction:

$$I_1^j(\varphi, \varphi^*) \equiv \int_a^b \left(\Psi + \Delta\tau^j \left(u\frac{\partial \Psi}{\partial x} - \frac{\partial}{\partial x}\mu\frac{\partial \Psi}{\partial x} + \mathrm{d}\Psi \right) - W \right) \varphi^* \mathrm{d}x = 0. \tag{14}$$

Here $x \in [a, b]$ is one of the co-ordinates in the domain D_t, $\Psi = \sigma\varphi^j + (1-\sigma)\varphi^{j-1}$, $W = \varphi^{j-1} + \Delta\tau^j f^j$, $\Delta\tau^j = \sigma\Delta t_j$, $\Delta t_j = t_j - t_{j-1}$, $0.5 \le \sigma \le 1$. A two-layer scheme is chosen for time discretisation. This leads to explicit–implicit weighted schemes [29]. If $\sigma = 0.5$, this is the Crank–Nicolson scheme with the accuracy of $o(\Delta t)^2$. If $\sigma = 1$, this is the first order implicit scheme. After finding the function Ψ, the sought function φ^j is calculated by the formula

$$\varphi^j = \frac{1}{\sigma}\left(\Psi - (1-\sigma)\varphi^{j-1}\right). \tag{15}$$

3. A hybrid discretisation scheme

The integral identity of the model in variational form can be considered as the global balance relation weighted with adjoint functions. To construct the numerical schemes, we use the hybrid procedure, the main idea of which is as follows. In the domain $D_t^h = \left\{ S_{X_1}^h \times S_{X_2}^h \times S_{X_3}^h \times S_t^h \right\}$, the finite volume method defines the global structure of a 4D numerical model. Then the balance relation is constructed for each individual volume. The functions of two types that are sought, participate in this structure: the state functions and the adjoint weight functions. In the one-dimensional case they are:

$$\vec{\varphi} = \left\{ \varphi_i = \varphi(x_i), x_i \in S_{X_1}^h \subset D_t^h, i = \overline{1, n} \right\} \in Q^h(D_t^h), \tag{16}$$

$$\vec{\varphi}^* = \left\{ \varphi_i^* = \varphi^*(x_i), x_i \in S_{X_1}^h \subset D_t^h, i = \overline{1, n} \right\} \in Q^{*h}(D_t^h). \tag{17}$$

The remaining variables parametrically participate in the definitions. Internal links between the values of the functions φ_i and φ_i^* are defined by means of analytical solutions of the adjoint problems generated by the variational principle. In terms of (14) and (15), this is the family of the local adjoint problems defined on the set of grid cells $S_{X_1}^h$: $\left\{ x_i \le x \le x_{i+1}, (i = \overline{1, n-1}) \right\}$. They have the parametrically given conditions at the cell boundaries.

3.1. The internal structure of the numerical schemes

Let us form the internal structure of the numerical model. Denote

$$(L\Psi)_i \equiv \left(\Psi + \Delta\tau^j \left(u\frac{\partial \Psi}{\partial x} - \frac{\partial}{\partial x}\mu\frac{\partial \Psi}{\partial x} + \mathrm{d}\Psi \right) \right)_i, \tag{18}$$

$$(L^*\varphi^*)_i \equiv \left(\varphi^* + \Delta\tau^j \left(-u\frac{\partial \varphi^*}{\partial x} - \frac{\partial}{\partial x}\mu\frac{\partial \varphi^*}{\partial x} + \mathrm{d}\varphi^* \right) \right)_i, \tag{19}$$

$$U_i(\Psi, R, \varphi^*) = \left(\mu\Delta\tau^j \left(-\varphi^*\frac{\partial \Psi}{\partial x} + \Psi\frac{\partial \varphi^*}{\partial x} + \frac{u}{\mu}\Psi\varphi^* \right) \right)_i \Bigg|_{x_i}^{x_{i+1}} - R_i, \tag{20}$$

$$R_i = \int_{x_i}^{x_{i+1}} \left(W\varphi^*(x) \right)_i \mathrm{d}x. \tag{21}$$

The low index i shows that the correspondent object is defined within the cells $S_{X_1}^h = \{[x_i \le x \le x_{i+1}], \Delta x_i = x_{i+1} - x_i, (i = \overline{1, n-1}), x_1 \equiv a, x_n \equiv b\}$ in the time interval $\left[t_{j-1}, t_j\right]$. In the splitting method, the main operator and formally adjoint to it, the differential operator are denoted as $(L\Psi)_i$ and $(L^*\varphi^*)_i$, respectively; R_i are the integrals of the source function W at the step $\left[t_{j-1}, t_j\right]$, $U_i(,,)$ are the bilinear forms of Ψ and φ^*. In the forms $U_1(,,)$ for $x = x_1$ and $U_{n-1}(,,)$ for $x = x_n$ the derivatives $\partial\Psi/\partial x$ are excluded by means of boundary conditions (4) if $\gamma = 1$. In what follows, this will provide the automatic accounting of Neumann and Robin boundary conditions. If $\gamma = 0$, Dirichlet conditions are taken into consideration in an ordinary way. The functions μ, u, d, R participate as parameters. To present these parameters in the system of finite volumes, we use a piecewise constant approximation of the second order in the sense:

$$(a)_i \equiv a_{i+1/2} = \frac{1}{\Delta x_i}\int_{x_i}^{x_{i+1}} a(x)\mathrm{d}x \approx 0.5\,(a_{i+1} + a_i). \tag{22}$$

Choosing such approximation of parameters, we write the fitting conditions for the state functions at the cell boundaries as

$$(\mu)_{i-1}\left.\frac{\partial\Psi}{\partial x}\right|_{i-0} = (\mu)_i\left.\frac{\partial\Psi}{\partial x}\right|_{i+0}, \quad \Psi|_{i-0} = \Psi|_{i+0}. \tag{23}$$

For the periodic case we put $\Psi_n = \Psi_1$ at the boundaries of the domain D_t^h.

Direct fitting of the advective fluxes $(u)_{i-1}\,\Psi|_{i-0}$ and $(u)_i\,\Psi|_{i+0}$ is not carried out at the cell boundaries. The required adjustment is provided by the use of the discrete analogue of the continuity equation (3) simultaneously approximated along all three directions (X_1, X_2, X_3) at the grid points of the domain D_t^h. The piecewise constant approximation of the parameters (22) is chosen exactly for fitting with the balanced approximation of the continuity equation. That is why the approximations of the transport operators in all directions should be built in the same way. If the continuity equation is in the form (3) having $\pi \neq const$, then the sets of parameters $(\mu, u, d, R)_i$ should be changed to $(\mu\pi, u\pi, d\pi, R\pi)_i$ everywhere. The conditions at the external boundaries are given under (4). Taking into account the accepted notations, the functional (14) is written in the form

$$\begin{aligned} I_1^{hj}(\Psi, \varphi^*) &= \sum_{i=1}^{n-1}\int_{x_i}^{x_{i+1}} (L\Psi - W)_i\,\varphi_i^*(x)\mathrm{d}x \\ &= \sum_{i=1}^{n-1}\left\{\int_{x_i}^{x_{i+1}} \left(L^*\varphi^*\Psi\right)_i \mathrm{d}x + U_i(\Psi, R, \varphi^*)\right\} = 0. \end{aligned} \tag{24}$$

Eq. (24) expresses the weighted balance relation over the range of the variable x. On one hand, if the value of the functional $I_1^{hj}(\Psi, \varphi^*)$ is required to be stationary with respect to the variations of the trial functions $\varphi^*(x)$ in each cell, we obtain the set of the local balance relations

$$(L\Psi - F)_i = 0, \qquad x_i \le x \le x_{i+1}, \quad \Psi(x_i) = \Psi_i, \qquad \Psi(x_{i+1}) = \Psi_{i+1}; \tag{25}$$

$$\int_{x_i}^{x_{i+1}} (L\Psi - W)_i\,\varphi_i^*(x)\mathrm{d}x = \int_{x_i}^{x_{i+1}} \left(L^*\varphi^*\Psi\right)_i \mathrm{d}x + U_i(\Psi, R, \varphi^*) = 0. \tag{26}$$

On the other hand, if the stationary conditions are demanded to be fulfilled with respect to the variations of Ψ in the cells, we get the balance relation from (26) in the form

$$\int_{x_i}^{x_{i+1}} (L\Psi - W)_i\,\varphi_i^*(x)\mathrm{d}x = U_i(\Psi, R, \varphi^*) = 0. \tag{27}$$

The simultaneous fulfilment of (25)–(27) gives the base for an optimal choice of the adjoint functions satisfying the equation

$$\left(L^*\varphi^*\right)_i = 0, \quad i = \overline{1, n-1}. \tag{28}$$

Thus, the optimality of the numerical schemes is meant in the sense that the value of functional (24) is bistationary with respect to the first order variations of the functions $\delta\varphi^*$ and $\delta\Psi$. As each fragment satisfies the requirements of bistationarity, the objects (13) and (14) possess the same property in a whole.

Let us describe the scheme of construction of the optimal weight functions with the use of local adjoint problems (28). Define the set of fundamental solutions of the problems with the specific conditions at the cell boundaries

$$L_i^*\omega_i^{(\alpha)}(x) = 0, \quad \alpha = 1, 2, \quad x_i \le x \le x_{i+1}, \quad i = \overline{1, n-1}; \tag{29}$$

$$\begin{aligned} &(1)\ \omega_i^{(1)}(x_i) = 0; \qquad \omega_i^{(1)}(x_{i+1}) = 1; \\ &(2)\ \omega_i^{(2)}(x_i) = 1; \qquad \omega_i^{(2)}(x_{i+1}) = 0. \end{aligned} \tag{30}$$

In other words, the analytical solutions of two boundary problems are constructed for each cell:

$$\omega_i^{(1)}(x) = A_i\left(\mathrm{e}^{-\nu_1 x'} - \mathrm{e}^{\nu_2(1-x')-\nu_1}\right),$$

$$\omega_i^{(2)}(x) = A_i\left(\mathrm{e}^{\nu_2(1-x')} - \mathrm{e}^{\nu_2-\nu_1 x'}\right),$$

$$x' = (x_{i+1} - x)/\Delta x_i, \quad A_i = \left(1/(1 - \mathrm{e}^{(\nu_2-\nu_1)})\right)_i.$$

Here $\{\nu_1 = \lambda_1\Delta x, \nu_2 = \lambda_2\Delta x\}_i$ where $\{\lambda_1 \ge 0, \lambda_2 \le 0\}_i$ are the non-negative and non-positive roots of the characteristic equations of the formally adjoint operators $(L^*\varphi^*)_i = 0$ from (28). These equations

$$\left\{\lambda^2 + \frac{u}{\mu}\lambda - \frac{1 + d\Delta\tau}{\mu\Delta\tau} = 0\right\}_i^j \tag{31}$$

are defined in the intervals $x_i \le x \le x_{i+1},\ i = \overline{1, n-1},\ j = \overline{1, J}$ on the supposition that the parameters are real and constant within the intervals: $\mu > 0, d \ge 0$, u can be of different signs, $|u| \ge 0$. The found fundamental solutions to the problems (29) and (30) are used to form n weight functions for organising a three-point approximation on the grid structure (17)

$$\begin{aligned}
&\varphi_i^*(x) = \varphi_i^* \omega_i(x), \quad i = \overline{1, n};\\
&\omega_i(x) = \begin{cases} \omega_{i-1}^{(1)}(x) & x_{i-1} \le x \le x_i, \\ \omega_i^{(2)}(x) & x_i \le x \le x_{i+1}, \end{cases} \ i = \overline{2, n-1};\\
&\omega_1(x) = \omega_1^{(2)}(x), \quad x_1 \le x \le x_2; \quad \omega_n(x) = \omega_{n-1}^{(1)}(x), \quad x_{n-1} \le x \le x_n.
\end{aligned} \tag{32}$$

Then from (24) using the definition of the weight functions $\varphi_i^*(x)$ (32) and the conditions (29), we get the equation

$$\begin{aligned}
I_1^j(\Psi, \varphi^*) &= \sum_{i=2}^{n-1} \varphi_i^* \left[U_{i-1}\left(\Psi, R, \omega^{(1)}(x)\right) + U_i\left(\Psi, R, \omega^{(2)}(x)\right)\right] + \varphi_1^* U_1\left(\Psi, R, \omega^{(2)}(x)\right) + \varphi_n^* U_{n-1}\left(\Psi, R, \omega^{(1)}(x)\right)\\
&= 0.
\end{aligned} \tag{33}$$

Numerical schemes are obtained from the stationary conditions for the functional (33), with respect to arbitrary and independent variations of the weight functions $\varphi_i^* = \varphi_i^*(x_i)$ at the grid points $x_i,\ i = \overline{1, n}$:

$$\begin{aligned}
&U_{i-1}\left(\Psi, R, \omega^{(1)}(x)\right) + U_i\left(\Psi, R, \omega^{(2)}(x)\right) = 0, \quad \left(i = \overline{2, n-1}\right),\\
&U_1\left(\Psi, R, \omega^{(2)}(x)\right) = 0, \quad (i = 1); \qquad U_{n-1}\left(\Psi, R, \omega^{(1)}(x)\right) = 0, \quad (i = n).
\end{aligned} \tag{34}$$

Relations (34) are a system of equations for finding the functions Ψ_i in the grid nodes in accordance with (16). Now, let us transform the equations of the system (34), taking into account the forms $U_i(,,)$ from (20), the consistency conditions (23) for the state functions, and the analytical formulas for the weight functions from (32). Neumann and Robin conditions at the external boundaries are taken into account via the forms $U_i(,,)$ for $i = 1, n-1$. Dirichlet conditions give the known boundary values for Ψ_1 and Ψ_n. In the periodic case, we put $\Psi_1 = \Psi_n$ and sum the equations for $i = 1$ and $i = n$. Their sum gets the number $i = 1$.

Finally, we obtain the usual three-point system of equations for finding the functions Ψ_i at the grid points x_i over the time interval $[t_{j-1}, t_j], j = \overline{1, J}$:

$$-c_i\Psi_{i-1} + b_i\Psi_i - a_i\Psi_{i+1} = F_i, \quad i = \overline{1, n}; \tag{35}$$

$$\begin{aligned}
&c_1 = 0, \qquad c_i = S_{i-1}\left(\mathrm{e}^{-\nu_1}\eta(\nu_1 - \nu_2)\right)_{i-1}, \quad i = \overline{2, n},\\
&a_n = 0, \qquad a_i = S_i\left(\mathrm{e}^{\nu_2}\eta(\nu_1 - \nu_2)\right)_i, \quad i = \overline{1, n-1},\\
&b_1^- = 0, \qquad b_i^- = S_{i-1}\left(\eta(\nu_1 - \nu_2) - \nu_1\right)_{i-1}, \quad i = \overline{2, n},\\
&b_n^+ = 0, \qquad b_i^+ = S_i\left(\eta(\nu_1 - \nu_2) + \nu_2\right)_i, \quad i = \overline{1, n-1},\\
&b_i = b_i^- + b_i^+; \qquad F_i = F_i^- + F_i^+; \quad F_i^- = (W)_{i-1} I_i^-; \quad F^+ = (W)_i I_i^+;\\
&I_1^- = 0, \qquad I_i^- = (A\Delta x)_{i-1}\left(\xi(\nu_1) - \mathrm{e}^{-\nu_1}\xi(\nu_2)\right)_{i-1}, \quad i = \overline{2, n},\\
&I_n^+ = 0, \qquad I_i^+ = (A\Delta x)_i\left(\xi(-\nu_2) - \mathrm{e}^{\nu_2}\xi(\nu_1)\right)_i, \quad i = \overline{1, n-1},\\
&S_i \equiv (\mu\Delta\tau/\Delta x)_i;\\
&\eta(\nu) = \begin{cases} \nu/\left(1 - \mathrm{e}^{-\nu}\right), & \nu > 0; \\ 1, & \nu = 0; \end{cases} \qquad \xi(\nu) = \begin{cases} 1/\eta(\nu), & \nu > 0; \\ 1, & \nu = 0; \end{cases}
\end{aligned}$$

$$\varphi_i^j = \left(\Psi_i - (1-\sigma)\,\varphi_i^{j-1}\right)/\sigma, \quad i = \overline{1, n}. \tag{36}$$

If $\nu \le \varepsilon$, the approximate formula of $o(\nu^4)$ can be used

$$\eta(\nu) = 1/\left((1 - \nu/4)^2 + (5/48)\,\nu^2\right).$$

For the Dirichlet problem, the equations are solved for $i = \overline{2, n-1}$. In periodic case, the number of equations is $i = \overline{1, n-1}$. Due to boundary conditions (4), there are additional terms in the coefficients b_1^+ and I_1^+, b_n^- and I_n^- in the cases of Neumann and Robin conditions. The automatic orientation of the scheme (35) with respect to the signs of eigenvalues of (31) provides the transportivity and monotony of the processes if the velocity component changes its sign.

3.2. Algorithm for the construction of adjoint problems

Following the algorithm from Section 2.4, the numerical schemes for the adjoint problems are constructed on the base of the extended functional (11) by analogy with (33)–(36). Writing down the stationary conditions for the fragment of the

functional (11) corresponding (14) with respect to the variation of φ_i^j, we obtain the adjoint system in the form

$$\varphi_i^{*j} = \frac{1}{\sigma}\left[\left(I_i^- + I_i^+\right)^{j+1}\Psi_i^{*j+1} + (1-\sigma)\,\varphi_i^{*j+1} - \frac{\partial \Phi^j\left(\vec{\varphi}, \vec{Y}\right)}{\partial \varphi_i^j}\right], \tag{37}$$

$$\begin{aligned} &\left\{-a_{i-1}\Psi_{i-1}^* + b_i\Psi_i^* - c_{i+1}\Psi_{i+1}^* + \varphi_i^*\right\}^j = 0; \\ &\Psi_i^{*J+1} = 0; \quad \varphi_i^{*J+1} = 0; \quad i = \overline{1, n}; \quad j = \overline{J, 1}; \quad a_0^j = 0; \quad c_{N+1}^j = 0. \end{aligned} \tag{38}$$

The adjoint systems are solved backward in time. The boundary conditions are taken into account in the structure of the sum analogues of the functional. They are written as the consequence of the conditions in (33)–(35). If $\sigma = 1$, the adjoint implicit scheme is produced. And if $\sigma = 0.5$, the Crank–Nicolson scheme is obtained. The schemes (35), (36) and (37), (38) are the interrelated basic algorithms for direct and inverse modelling.

3.3. Quality analysis of the numerical schemes

The following Theorem is valid. If the parameters satisfy the conditions $\mu > 0$, $d \geq 0$, $|u| \geq 0$, then the numerical scheme (35) possesses the properties:

1. The coefficients satisfy the conditions
$$\left\{c_i \geq 0, \quad a_i \geq 0, \quad b_i > 0, \quad b_i^- \geq c_i, \quad b_i^+ \geq a_i\right\}, \quad i = \overline{1, n}. \tag{39}$$
2. The matrix of the coefficients is of tridiagonal structure with strong diagonal predominance. The inverse matrix exists and has non-negative elements.
3. When $\sigma = 1$, the numerical scheme is absolutely stable, monotone and transportive by any ratio of the parameters of the grid domain.

Item 1 is checked at once. The fulfilment of Items 2 and 3 are immediate corollaries of Item 1. They are proved by the use of the theorems about the properties of monotonic matrices [4,33]. If $\sigma = 0.5$, the scheme (35) is of the second order in time, i.e. $o(\Delta t^2)$. As all constructions with respect to the horizontal variable are made analytically, the order of approximation is defined by the accuracy of assignment of both the parameters and the right side of the equations in the grid cells. In the considered case, this is $o(\Delta x^2)$ even if the grid is non-uniform.

If the parameter $d(x, t)$ is negative everywhere or somewhere in x within the time interval $t_{j-1} \leq t \leq t_j$, first of all it is necessary to change to the new state functions $\tilde{\varphi}$ by means of the formula $\varphi = \mathrm{e}^{\tilde{\lambda}t}\tilde{\varphi}$, where $\tilde{\lambda} = \max_{\langle x|d(x)<0\rangle} |d(x, t)|$. Then all operations are carried out by the above described scheme of implicit algorithm with parameters $\tilde{d} = \tilde{\lambda} + d, \tilde{f} = f\mathrm{e}^{-\tilde{\lambda}t}$. Finally, the result is presented in the terms of Ψ and φ. This approach allows the problems with physically unstable states to be solved by means of stable and monotonic schemes. It is worth remembering that if $\gamma \geq 0$ and $\beta \geq 0$ (the simultaneous equality to 0 is excluded) along all co-ordinates, the operators of the model (18) and (19) with boundary conditions (4) belong to the class of linear differential operators of monotonic type [4]. The described methodology for constructing numerical schemes maintains the monotonicity property in the discrete approximations of the forward and adjoint versions. This is a fundamental result for numerical transport-diffusion modelling. In essence, the use of the local adjoint problem technique in the variational principle, is a new universal tool for the construction of discrete analogues of differential operators without finite differences. It should be emphasized that the schemes obtained are linear with respect to both the state and adjoint functions.

The limiting factor of applicability, even for absolutely stable implicit schemes, is the condition of approximation. For advective-diffusive problems this condition can be estimated by means of the Courant–Friedrichs–Levi criterion

$$CFL = \max_{\langle i\rangle}\left\{\frac{|u|\,\Delta\tau}{\Delta x} + \frac{2\mu\Delta\tau}{\Delta x^2} + d\Delta\tau\right\}_i < 1. \tag{40}$$

With these conditions being fulfilled, all explicit–implicit schemes ($\sigma \geq 0.5$) hold the monotonicity property. For explicit schemes built by our technology, the approximation condition (40) also ensures the monotonicity and stability. But even if the CFL criterion is valid, the adequate description of the processes will be provided only if the ratio between the turbulent and convective parts of the operator is correct. Such a consistent description is provided if the condition

$$\max\left\{(\nu_1 - \nu_2)_i, (R_{cell})_i\right\} \leq B_c, \tag{41}$$

is satisfied. Here $R_{cell} = |u|\,\Delta x/\mu$ is the cell Reynolds number. The value of B_c is chosen from the significance limits of the exponential functions included in the coefficients and right side in the scheme (35). For example, it follows that $B_c \leq 10$ for a computer with 32-bit arithmetic. The value R_{cell} is used for the assessment of numerical scheme applicability for advective-diffusive problems. As it is mentioned in [6], the parameter $B_c < 10$ is in use for the most popular numerical schemes. Moreover, the restriction $R_{cell} \leq 2$ has to be fulfilled to get monotonicity and convergence for them [28].

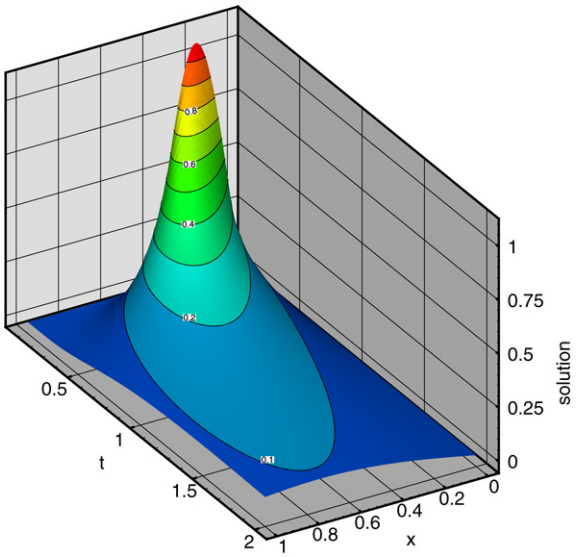

Fig. 1. The solution obtained by the Crank–Nicolson scheme.

As all operations for construction of the scheme (35) are analytically produced, there is no problem with artificial numerical diffusion in our schemes. Such a problem arises if the monotonic schemes are constructed by finite differences. Our scheme preserves its properties when $\mu \to 0$ and $R_{cell} \to \infty$. However, the procedures for the calculation of the coefficients and the right sides in (35) should be correctly organised while approaching the limits. If $\mu \to 0$, the scheme (35) changes into the transportive, absolutely monotonic and stable balanced scheme that approximates the transport operator. It is still consistent with the divergence approximation in the continuity equation (3).

4. Numerical test

To test the quality of numerical schemes, we consider an example of the Dirichlet boundary problem for the non-stationary non-linear Burgers equation

$$\frac{\partial \varphi}{\partial t} + \varphi \frac{\partial \varphi}{\partial x} - \mu \frac{\partial^2 \varphi}{\partial x^2} = 0. \tag{42}$$

The equations of such type are traditionally used for testing the algorithms in numerical fluid dynamics [6]. An example have been taken from the recent paper [2].

Example. Consider the solution of the Eq. (42) in the domain $D_t = \{0 \le x \le 1, 0 \le t \le 2\}$ with the given initial and boundary conditions $\varphi(x, 1)$, $\varphi(0, t)$, $\varphi(1, t)$. The values of these functions are calculated from the formula for the exact solution

$$\varphi(x, t) = x \left[t \left(1 + \sqrt{t} \exp\left(x^2 / (4\mu t) \right) \right) \right]^{-1}. \tag{43}$$

Following [2], the variant with $\mu = 0.1$ is calculated. Two versions of the scheme (35) are tested : with $\sigma = 1$ (implicit) and with $\sigma = 0.5$ (Crank–Nicolson). In both cases the linearization of the advective terms is made with respect to the solution at the previous time step. The grid domain is of 201×101 points in space and time, respectively. In Fig. 1, the solution obtained by the Crank–Nicolson scheme is given. The errors for both schemes are shown in Fig. 2. They characterise the difference between the exact $\varphi(x_i, t_j)$ and the approximate φ_i^j solutions calculated by the formula

$$e_2 \equiv \left\{ e_2^j, j = \overline{1, J} \right\} = \left(\sum_{i=1}^{n} \Delta x_i \left(\varphi(x_i, t_j) - \varphi_i^j \right)^2 \right)^{1/2}. \tag{44}$$

5. Assessment of risk for Lake Baikal

The environmental modelling methodology is intended for the solution of a wide range of problems. Its advantage is that it allows us to consistently solve both the direct (forward) and the inverse problems. Some examples for the application of the methodology to the solution of typical problems for the assessment of the ecological future of industrial regions are presented in [24–27].

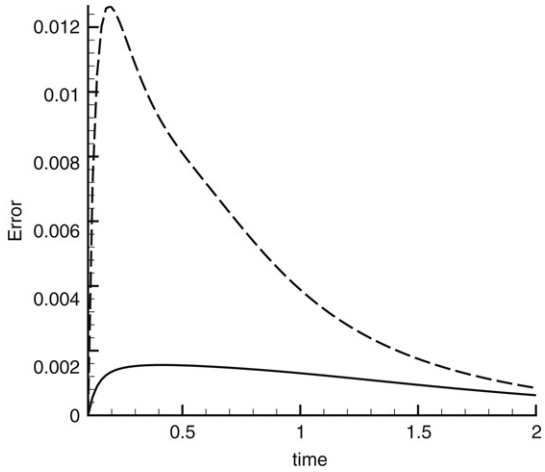

Fig. 2. The errors calculated by (44) for the Crank-Nicolson scheme (solid line) and for the first order scheme (dashed line)

In this section, we consider an example of inverse modelling. The goal of the scenario is to assess the degree of risk for Lake Baikal, to obtain contamination from all possible sources in the region. The region including the lake is situated in the southern part of Eastern Siberia, Russia. For calculations, the set of environmental models CARMEN (Complex of Atmospheric Regional Models for Environmental Needs) being developed by us, is used. A version of the complex adopted to the Lake Baikal region is described in [22]. To calculate this particular scenario, a new version of numerical models is taken. The above mentioned discrete-analytical schemes for the solution of the forward and adjoint problems are involved there. The scenario is realised for the conditions of the regional climatic system behaviour in August, 2005. Below we shortly describe the conditions of the scenario.

1. The regions D_t and D_t^h are described as follows. The spherical horizontal co-ordinates are taken, $(47, 5°N–60°N, 95°E–115°E)$. The vertical scale ranges from the Earth surface to the 10-hPa level. A hybrid $(\sigma\text{-}p)$ co-ordinate following the Earth surface is chosen. The resolution of the grid domain is $(0.25° \times 0.25°)$ along the horizontal co-ordinates and 19 vertical levels. The time interval is from 00:00 GMT 1.08.2005 to 00:00 GMT 1.09.2005. The basic time step is 30 min. The actual time step depends on the CFL conditions (40).

2. The scenario is realised in the inverse mode with the given goal functional (8). It is formed so that $F_k \equiv \varphi(\vec{X}, t)$, where φ is the concentration of a passive substance in the atmosphere. The weight function χ_k is given in such a way that the carrier of its non-zero values describes the region-receptor above the lake : $D_{Lt}^h = \{(X_1, X_2) \in S_L\}$, where S_L is the surface of the lake. The range of the vertical co-ordinate and the time interval are the same as in D_t. The value of the functional is the total monthly amount of pollution which is able to enter into the air column over the lake, due to the action of possible sources in the region or from trans-boundary transport.

3. The hydrodynamic part of the scenario is formed with the use of reanalysis data [9]. The 4D fields of meteorological elements and other necessary parameters are calculated on the base of this information. The regional model and the 4D data assimilation system being in the model set are used for this goal.

4. To assess the risk we need the values of the sensitivity functions of the goal functional (8) to the variations of the sources $f(\vec{X}, t)$ emitting the substance φ. The source term is explicitly included in the model description (1), (2). Denote the sensitivity functions by $SF(f)$ and define its sense and the algorithm for its calculation as

$$SF(f) = \frac{\partial}{\partial f(\vec{X}_i, t_j)} \Phi^h(\varphi) = \frac{\partial I^h(\varphi, \varphi^*)}{\partial f(\vec{X}_i, t_j)}, \quad \left(\vec{X}_i, t_j\right) \in D_t^h. \tag{45}$$

It is seen that $SF(f)$ has a 4D space-time structure. Its values show which part of the total emission from the sources may enter into the receptor zone. The greater the value of $SF(f)$ at a grid point, the more the risk to get the input into the quality functional from the source situated at this point. All necessary algorithms for the scenario are formed on the base of the augmented functional (11). Following the scheme of the universal algorithm of the direct and inverse modelling, the adjoint problems (37) and (38) are solved backward in time and then the SFs are calculated by (45). Analysing the scenario as a whole, we should make the conclusion that the industrial areas concentrated near the big cities in the East-Siberian region are the zones of the increased risk for Lake Baikal. The calculated SFs show high variability in space and time. This is demonstrated in Fig. 3 in which the 2D fragments related to the time moments of 18:30 GMT 03.08.2005 (left) and 21:00 GMT 19.08.2005 (right) are drawn. The field of $\vec{u}$ (arrows, m/s) at the upper boundary of the surface layer and the sensitivity function (isolines, relative units) to the variations of the power of sources located at the Earth's surface in the region and beyond it, are presented. It is seen that pollution may come from the north-west direction as in Fig. 3 (left) or from the north-west and south-east directions as in Fig. 3 (right). A significant part of the risk domain falls into the

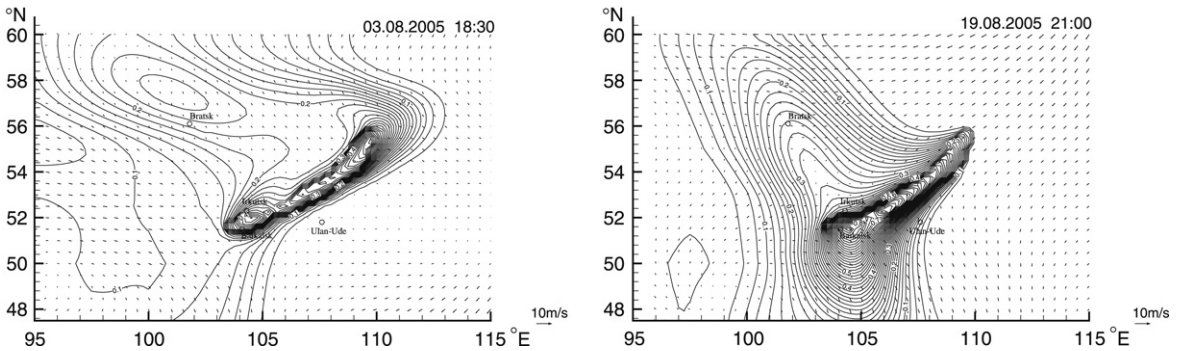

Fig. 3. Two-dimensional sections of the velocity fields (arrows) and the isolines of the sensitivity (risk) functions for the receptor at the level corresponding to the surface layer height at the time moments: 18:30 GMT 03.08.2005 (left) and 21:00 GMT 19.08.2005 (right).

Mongolia territory. The results of such scenarios are useful to design environment protection strategies and observational programmes.

6. Conclusion

The new method proposed above for constructing numerical schemes for convection-diffusion problems is based on a variational principle with the discrete-analytical approximations. The use of the local adjoint problem technique in the framework of the variational principle is, in essence, a universal tool for the construction of discrete analogues of differential operators without finite differences. The new schemes are absolutely stable, monotonic, transportive, and very simple and efficient in algorithmic realisation. Including analytical solutions, prevents the occurrence of artificial diffusion. The variational technique guarantees that there is exact consistency between the main and adjoint problems. This property is important for the realisation of direct and inverse methods of numerical modelling in the atmosphere, ocean, and the environment.

Acknowledgements

We are grateful to the reviewers for their comments. This research was supported by Program 16 of RAS, Program 3 of the Mathematical Sciences Department of RAS, RFBR grant 07-05-00673, and European Commission contract N 013427.

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